

# Relativistic Oscillator Strengths in Chlorine

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## 1 Introduction

Models of interstellar chlorine chemistry can be used to constrain models of interstellar clouds. One difficulty in confirming the basic ideas of this model is that the analyses have been based on rather poorly known oscillator strengths for *Cl I*, as has been emphasized by Keenan & Dufton [1] and Morton [2]. We have followed the Relativistic Quantum Defect Orbital (RQDO) procedure [3] with and without explicit inclusion of core-valence correlation. The observations [4] of the *Cl I* spectrum show that LS coupling is valid for the deepest  $3p^4$  ns, np and nd configurations whereas pair coupling is progressively better satisfied for higher  $l$  and  $n$  values. In our calculations of oscillator strengths, we have followed the LS coupling scheme, except for the  $3p^4(^3P)4f - 3p^4(^3P)5g$  lines, for which the  $J_c I$  coupling scheme seems clearly to be more appropriate.

## 2 Method of Calculation

The absorption oscillator strength for an electric dipole transition between an initial state,  $|i\rangle$ , and a final state,  $|j\rangle$ , is given by

$$f_{ij} = \frac{2}{3} \frac{(E_j - E_i)}{2J + 1} S \quad (1)$$

where  $(E_j - E_i)$  is the transition energy (in atomic units),  $2J + 1$  is the degeneracy of the initial level and  $S$  is the so-called line strength (in atomic units). In a one-configuration treatment, such as ours, the angular and radial parts of the line strength can be separated. Within *LS* coupling, the line strength is written as follows:

$$S(\gamma SLJ, \gamma' S'L'J') = \left| \delta_{SS'} \delta_{cc'} R_{line}(SLJ, S'L'J') R_{mult}(\gamma L, \gamma' L') (-1)^{J-L} \sqrt{J} \int R_{nl}(r) R_{n'l'}(r) r dr \right|^2 \quad (2)$$

where  $J$  and  $J'$ ,  $L$  and  $L'$ ,  $S$  and  $S'$ , and  $\gamma$  and  $\gamma'$  represent the quantum numbers required to complete the specification of the states  $|i\rangle$  and  $|j\rangle$ , respectively. The subscripts  $c$  and  $c'$  refer to the core. The integral in (2) contains the radial parts of the initial and final wavefunctions only. The line factor,  $R_{line}$ ,

$$R_{line} = \sqrt{2J+1} \sqrt{2J'+1} (-1)^{S+J+L+1} \begin{Bmatrix} S & J & L \\ 1 & L' & J' \end{Bmatrix} \quad , \quad (3)$$

is given by the above expression, where the symbol in braces is a  $6-j$  symbol.  $(R_{line})^2$  gives the relative strength of the lines within a multiplet. In (2),  $nl$  and  $n'l'$  are, respectively, the principal and orbital angular momentum quantum numbers of the jumping electron, and  $l_>$  indicates the larger of the two orbital quantum numbers,  $l$  and  $l'$ , involved in the transition.

The multiplet factor,  $R_{mult}$  depends upon the particular configurations involved in the transition:

- for  $3s^2 3p^4 nl - 3s^2 3p^4 n'l'$  the multiplet factor adopts the form

$$R_{mult} = \sqrt{2L+1} \sqrt{2J'+1} (-1)^{L_c+L+I+1} \begin{Bmatrix} L_c & l & L \\ 1 & l' & I' \end{Bmatrix} \quad (4)$$

-and for  $3s^2 3p^5 - 3s^2 3p^4 n'l'$  the multiplet factor is

$$R_{mult} = \sqrt{5} \sqrt{2L+1} \sqrt{2L'+1} (-1)^{L_c+L+I+1} \begin{Bmatrix} L_c & l & L \\ 1 & l' & I' \end{Bmatrix} (p^5 LS \{ | p^4 (L_c S_c) pLS \}) \quad (5)$$

where  $(p^5 LS \{ | p^4 (L_c S_c) pLS \})$  is the coefficient of fractional parentage, CFP.

The expression for the line strength in the  $J_c l$  coupling scheme is

$$S = (2J+1)(2J'+1) \left\{ \begin{matrix} K & \frac{1}{2} & J \\ J' & 1 & K' \end{matrix} \right\}^2 (2K+1)(2K'+1) \left\{ \begin{matrix} J_c & l & K \\ 1 & K' & I' \end{matrix} \right\}^2 l_> \left| \int R_{nl} R_{n'l'} r dr \right|^2 \quad (6)$$

where  $J_c$  is the total angular momentum quantum number of the electron core  $3p^4 {}^3P$  level;  $K$  results from the coupling of the orbital angular momentum,  $l$ , of the valence electron with  $J_c$  and  $J$  is obtained through the addition of the spin of the valence electron to  $K$ .

### 3 Results

#### **$3p^5 {}^2P^o - 3p^4 ({}^3P) 4s {}^2P$ Transitions**

Some lines of the  $3p^5 {}^2P^o - 3p^4 ({}^3P) 4s {}^2P$  multiplet of neutral chlorine have been the object of several theoretical studies, as well as measurements, because of their importance in astrophysics. Table 1 contains fine structure oscillator strengths for the  $3p^5 {}^2P^o - 3p^4 ({}^3P) 4s {}^2P$  transitions in  $CI I$ . In this table we display, together with the RQDO results [5], the f-values calculated by Biémont et al. [6] with the SUPERSTRUCTURE (SST) computer program, taking the most important configuration interaction and relativistic effects into account, as well as the results of Ojha & Hibbert [7], who used large multiconfiguration expansions in the atomic structure code CIV3. Biémont et al. and Ojha & Hibbert report f-values calculated in dipole length and velocity approaches.

The most accurate laboratory data are the measurements of Schectman et al. [8] using beam-foil spectroscopy. These authors estimated that their results should be accurate to about 7%. The present results, without explicit account for polarization, are in good accordance with the most accurate theoretical and experimental results. Our f-values for the  $3p^5\ ^2P_{3/2}^0 - 3p^4(^3P)4s\ ^2P_{3/2}$  and  $3p^5\ ^2P_{1/2}^0 - 3p^4(^3P)4s\ ^2P_{3/2}$  lines are larger than the earlier measurements for these transitions and confirm the recent experimental data of Schectman et al. For the remaining transitions, our f-values are in good accord with the measurements of Clyne & Nipp [9].

### **$3p^4(^3P)4f - 3p^4(^3P)5g$ Transitions**

In Table 2, we display RQDO f-values for  $3p^4(^3P)4f - 3p^4(^3P)5g$  transitions calculated in the  $JL$  coupling scheme [5]. No comparison data have been found in the literature. The level designations in this table are given according to the notation  $3p^4\ (^{2S+1}L_{J_c})\ n\ [K]_J$  where  $J_c$  is the total angular momentum quantum number of the electron core  $3p^4\ ^3P$  level;  $K$  results from the coupling of the orbital angular momentum,  $l$ , of the valence electron with  $J_c$ , and  $J$  is obtained through the addition of the spin of the valence electron to  $K$ . According to Quinet et al. [10], in pure  $JL$  coupling, the energies of a pair of levels for a given  $J_c$  should fall on a parabola when plotted against  $h=1/2[K(K+1) - J_c(J_c+1) - l(l+1)]$ . This approximation is verified in the cases of 4f and 5g electrons.

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Table 1: Oscillator strengths for the  $3p^5 - 3p^4(^3P)4s$  fine structure transitions in *CI I*.

	<b>RQDO<sup>a</sup></b>	<b>RQDO<sup>b</sup></b>	<b>SST<sup>c</sup></b>	<b>CIV3<sup>d</sup></b>	<b>CC<sup>e</sup></b>	<b>Experiment</b>
$3p^2P^o_{3/2} - 4s^2P_{3/2}$	0.1368	0.1281	0.147	0.1324	0.114	$0.100 \pm 0.030^f$ $0.109 \pm 0.010^g$ $0.153 \pm 0.011^h$
$3p^2P^o_{3/2} - 4s^2P_{1/2}$	0.0249	0.0240	0.0299	0.0264	0.0233	$0.028 \pm 0.006^f$
$3p^2P^o_{1/2} - 4s^2P_{3/2}$	0.0561	0.0523	0.0530	0.0474	0.0418	$0.038 \pm 0.006^f$ $0.055 \pm 0.004^h$
$3p^2P^o_{1/2} - 4s^2P_{1/2}$	0.1017	0.0980	0.116	0.1051	0.088	$0.093 \pm 0.016^f$

<sup>a</sup>RQDO without explicit polarization correction [5]; <sup>b</sup>RQDO with explicit polarization correction [5]; <sup>c</sup>Biémont et al. [6], length form; <sup>d</sup>Ojha & Hibbert [7], length form <sup>e</sup>Critical compilation, Wiese et al. [11]; <sup>f</sup>Clyne & Nipp [9]; <sup>g</sup>Schwab & Anderson [12]; <sup>h</sup>Schectman et al. [8].

Table 2: Oscillator strengths for the  $3p^4(^3P_2)4f [K]_J - 3p^4(^3P_2)5g [K]_J$  transitions in *CI I*.

	<b>RQDO<sup>a</sup></b>	<b>RQDO<sup>b</sup></b>		<b>RQDO<sup>a</sup></b>	<b>RQDO<sup>b</sup></b>
$[5]_{11/2} - [6]_{13/2}$	1.2217	1.2211	$[3]_{7/2} - [4]_{9/2}$	1.0697	1.0691
$[5]_{11/2} - [6]_{11/2}$	0.1031	0.1030	$[3]_{7/2} - [4]_{7/2}$	0.0307	0.0306
$[5]_{9/2} - [6]_{11/2}$	1.2354	1.2348	$[3]_{5/2} - [4]_{7/2}$	1.0989	1.0983
$[5]_{11/2} - [5]_{11/2}$	0.1031	0.1030	$[3]_{7/2} - [3]_{7/2}$	0.2247	0.2246
$[5]_{11/2} - [5]_{9/2}$	0.0016	0.0016	$[3]_{7/2} - [3]_{5/2}$	0.0083	0.0083
$[5]_{9/2} - [5]_{11/2}$	0.0019	0.0019	$[3]_{5/2} - [3]_{7/2}$	0.0111	0.0111
$[5]_{9/2} - [5]_{9/2}$	0.1028	0.1027	$[3]_{5/2} - [3]_{5/2}$	0.2220	0.2219
$[5]_{11/2} - [4]_{9/2}$	0.0040	0.0040	$[2]_{5/2} - [3]_{7/2}$	1.0668	1.0662
$[5]_{9/2} - [4]_{9/2}$	0.0001	0.0001	$[2]_{5/2} - [3]_{5/2}$	0.0532	0.0531
$[5]_{9/2} - [4]_{7/2}$	0.0040	0.0039	$[2]_{3/2} - [3]_{5/2}$	1.1201	1.1201
$[4]_{9/2} - [5]_{11/2}$	1.1263	1.1257	$[1]_{3/2} - [2]_{5/2}$	1.1216	1.1209
$[4]_{9/2} - [5]_{9/2}$	0.0209	0.0208	$[1]_{3/2} - [2]_{5/2}$	0.2691	0.2690
$[4]_{7/2} - [5]_{9/2}$	1.1481	1.1475	$[1]_{1/2} - [2]_{3/2}$	1.3466	1.3459
$[4]_{9/2} - [4]_{9/2}$	0.1802	0.1801	$[2]_{5/2} - [2]_{5/2}$	0.2051	0.2050
$[4]_{9/2} - [4]_{7/2}$	0.0041	0.0041	$[2]_{5/2} - [2]_{3/2}$	0.0149	0.0149
$[4]_{7/2} - [4]_{9/2}$	0.0052	0.0052	$[2]_{3/2} - [2]_{5/2}$	0.0224	0.0224
$[4]_{7/2} - [4]_{7/2}$	0.1794	0.1793	$[2]_{3/2} - [2]_{3/2}$	0.0897	0.0897
$[4]_{9/2} - [3]_{7/2}$	0.0093	0.0093			
$[4]_{7/2} - [3]_{5/2}$	0.0089	0.0089			
$[4]_{7/2} - [3]_{7/2}$	0.0004	0.0004			

<sup>a</sup>RQDO without explicit polarization correction; <sup>b</sup>RQDO with explicit polarization correction [3].